Flattening of Single-Particle Spectra in Strongly Correlated Electron Systems and the Violation of the Wiedemann-Franz Law

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The renormalization of the Wiedemann-Franz (WF) ratio in strongly correlated electron systems is analyzed within the Landau quasiparticle picture. We demonstrate that the WF law is violated: (i) at the quantum critical point, where the effective mass diverges, and (ii) beyond a point of fermion condensation, where the single-particle spectrum $\epsilon(p)$ becomes flat. Results of the analysis are compared with available experimental data.

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a. Introduction. In Landau theory,[1,2] a foundation of understanding of phenomena in condensed matter, Fermi liquid (FL) is treated as a system of interacting quasiparticles, having an ideal-Fermi-gas-like momentum distribution, (hereafter we set the Boltzmann's constant $k_B = 1$),

$$n(p) = \left[1 + e^{\epsilon(p)/T}\right]^{-1} . \qquad (1)$$

In the vicinity of the Fermi surface, the FL single-particle spectrum $\epsilon(p)$, measured from the chemical potential μ, also has the ideal-Fermi-gas form

$$\epsilon(p) = v_F(p - p_F) \equiv p_F(p - p_F)/M^* , \qquad (2)$$

where the bare mass M is replaced by a T-independent effective mass M^*. Therefore FL thermodynamic and transport properties differ from those of ideal Fermi gas merely by a numerical factor — a feature, inherent in atomic nuclei, liquid ^{3}He and conventional metals.

One of the most prominent justifications of the applicability of the Landau-Migdal quasiparticle picture to metals is associated with the low-temperature behavior of the Lorenz number $L(T)$, the ratio of the thermal conductivity $\kappa(T)$ to the product of temperature T and conductivity $\sigma(T)$. The $T \to 0$ limit L_0, derived by Sommerfeld well before the creation of FL theory, equals[3,4]

$$L_0 = \lim_{T\to 0} \frac{\kappa(T)}{\sigma(T)T} = \frac{\pi^2}{3e^2} . \qquad (3)$$

Eq. (3), known as the Wiedemann-Franz (WF) law, holds in normal states of electron systems of metals,[5,6,7,8,9] except for i) heavy-fermion metals[10,11,12] CeNiSn and $CeCoIn_5$, ii) an electron-doped material[13] $Pr_{2-x}Ce_xCuO_{4-y}$, and iii) an underdoped compound[14] $YbBa_2Cu_3O_y$. In CeNiSn, the experimental value of the reduced Lorenz number $L(T)/L_0 \simeq 1.5$ changes little at $T < 1\,\mathrm{K}$ that rules out the relevance of phonons to the violation of the WF law. In the electron-doped compound $Pr_{2-x}Ce_xCuO_{4-y}$, the departure of the ratio $L(T)/L_0$ from 1 at $T > 0.3\,\mathrm{K}$ is positive as well and even larger,[13] than in CeNiSn.

Predictions of FL theory, including Eq. (3), fail in the vicinity of the so-called quantum critical point (QCP) where the effective mass M^* diverges, since at the QCP, the FL spectrum (2) becomes meaningless. In a standard scenario of the QCP,[15,16] the divergence of the effective mass is attributed to vanishing of the quasiparticle weight z in the single-particle state close to points of second-order phase transitions, implying that the FL quasiparticle picture of phenomena breaks down. In dealing with the WF law, a scenario of its violation, associated with critical fluctuations, is recently advanced in Ref. 17. However, the standard scenario of the QCP is flawed,[18] and therefore in this article, we employ a different *topological* scenario of the QCP, where the departure of the Lorenz number $L(0)$ from the WF value is associated with a rearrangement of single-particle degrees of freedom, a phenomenon described within the Landau quasiparticle picture.

b. FL formulas for transport coefficients. Within Landau theory, relation between conductivities σ and κ, and the Seebeck thermoelectric coefficient S, has the form[3]

$$\frac{\kappa(T)}{\sigma(T)T} + S^2(T) = \frac{1}{e^2}\frac{I_2(T)}{I_0(T)} . \qquad (4)$$

Here

$$S(T) = \frac{1}{e}\frac{I_1(T)}{I_0(T)} , \qquad (5)$$

and

$$I_k(T) = -\int\left(\frac{\epsilon(p)}{T}\right)^k\left(\frac{d\epsilon(p)}{dp}\right)^2\tau(\epsilon,T)\frac{\partial n(p)}{\partial\epsilon(p)}d\upsilon, \qquad (6)$$

where τ is the collision time, $d\upsilon$ is the volume element of momentum space, and $n(p)$ is given by Eq. (1).

Overwhelming contributions to the integrals I_k come from a narrow vicinity $|\epsilon| \sim T$ of the Fermi surface. In Fermi liquids, obeying Landau theory, the Seebeck coefficient $S(T)$ vanishes linearly with T at $T \to 0$, similarly to the specific heat, given by

$$C(T) = -\int \epsilon(p)\frac{\partial n(p)}{\partial T}d\upsilon . \qquad (7)$$

Furthermore, in an ideal Fermi gas with impurities, the two quantities are connected with each other by relation[19]

$$q(T) = \frac{eS(T)N_{\rm Av}}{C(T)} = -1 \ , \qquad (8)$$

where $N_{\rm Av}$ is the Avogadro number. In interacting Fermi gases, the single-particle spectrum $\epsilon(p)$ is not a parabolic function of p, and $q(T) \neq -1$, nevertheless, the proportionality between $S(T)$ and $C(T)$ holds, and therefore the contribution of the Seebeck coefficient to Eq. (4) remains minor.

In conventional Fermi liquids, the group velocity can be factored out from the integrals (6). The same is valid for the collision time τ, depending at $T \to 0$ merely on impurity scattering. This yields[3,4] $I_1(T=0) = 0$, and $I_2(T \to 0)/I_0(T \to 0) = \pi^2/3$. Upon inserting these numbers into Eq. (4) we do arrive at Eq. (3) that holds, even if several bands cross the Fermi surface simultaneously.

It is worth noting that top-quality samples, used in modern experiments, possess an extremely low residual resistivity $\rho_0 < 0.5\mu\Omega$cm, and often at temperatures, at which measurements are carried out, electron-electron scattering comes into play, rendering the FL damping rate $\gamma \sim \tau^{-1}$ ϵ-dependent,[20]

$$\gamma(\epsilon, T) = \gamma(0,0) + \gamma_{ee}T^2(1 + (\epsilon/2\pi T)^2) \ , \qquad (9)$$

that alters the Lorenz number $L(T)$. To illustrate the change of its value we neglect the impurity scattering and set $\gamma(0,0) = 0$. In this case, the integrals I_k

$$I_k = -\frac{1}{\gamma_{ee}T^2}\int\Big(\frac{\epsilon}{T}\Big)^k\Big(\frac{d\epsilon}{dp}\Big)^2\frac{\partial n(\epsilon(p))}{\partial\epsilon}\frac{dv}{1+(\epsilon/2\pi T)^2} \qquad (10)$$

are calculated numerically, the results are inserted into Eq. (4) to yield

$$L(T)/L_0 = 0.84 \qquad (11)$$

that agrees with results obtained in Refs. 21,22 by a different method, giving rise to a slight decrease of $L(T)$ at temperatures where the resistivity $\rho(T)$ ceases to be constant. This suppression explains the departure of the experimental WF ratio from the FL value (3), found in the heavy-fermion metal $YbBa_2Cu_3O_y$.

c. Violation of the WF law at the topological quantum critical point. In homogeneous Fermi liquids, the QCP was uncovered first in experimental studies of a two-dimensional (2D) electron gas,[23,24,25,26] where the electron effective mass $M^*(\rho)$ diverges at a critical value $r_c \simeq 7.0$ of a dimensionless parameter $r_s = \sqrt{2}Me^2/p_F$. Results[27] of microscopic calculations of 2D electron spectra $\epsilon(p, T=0, r_s)$ at $r_s = 5$, 6 and 7 are shown in Fig. 1. We see that $\epsilon(p, T=0, r_s)$ becomes flatter and flatter, as the critical value $r_s = 7.0$ approaches, at which for the first time the group velocity $v = d\epsilon(p)/dp$ vanishes at the Fermi surface. As seen from Fig. 1, the QCP electron spectrum, denoted further $\epsilon_c(p, T=0)$, has an inflection point $\epsilon_c(p, T=0) \propto (p - p_F)^3$.

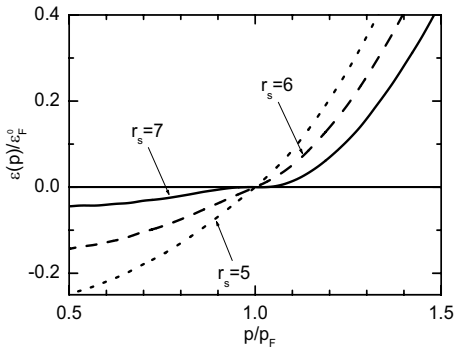

FIG. 1: Single-particle spectrum $\epsilon(p)$ of a homogeneous 2D electron gas in units of $\epsilon_F^0 = p_F^2/2M$, evaluated[27] at $T = 0$ for different values of the dimensionless parameter $r_s = \sqrt{2}Me^2/p_F$.

At finite T, the QCP group velocity $d\epsilon_c(p,T)/dp$ acquires a finite value,[28] and the QCP single-particle spectrum becomes[29]

$$\epsilon_c(p,T) = p_F\frac{p-p_F}{M^*(T)} + \frac{v_2}{3}(p-p_F)^3 \ . \qquad (12)$$

The T-dependence of the effective mass $M^*(T)$ is evaluated on the base of the Landau equation[1,2]

$$\frac{\partial\epsilon(p)}{\partial p} = \frac{p}{M} + \frac{1}{3}\int f_1(p,p_1)\frac{\partial n(p_1)}{\partial p_1}\frac{p_1^2 dp_1}{\pi^2} \ , \qquad (13)$$

connecting $\epsilon(p)$ with the quasiparticle momentum distribution $n(p)$, given by Eq. (1), in terms of the first harmonic f_1 of the interaction function f. If $f(q)$ is an analytical function of q, leading T-dependent contributions to $\epsilon(p,T)$ come from first terms of Taylor expansion of $f(p,p_1)$ vs $(p-p_F)$ and (p_1-p_F). As a result, one obtains[29]

$$\frac{M}{M^*(T)} = \left(\frac{9v_2}{8}\right)^{1/3}\left(\frac{TM}{p_F^2}\right)^{2/3} \ . \qquad (14)$$

To evaluate the integrals I_k, we introduce a new integration variable $\epsilon(p)$ instead of p, then express $p - p_F$ in terms of energy ϵ from Eq. (12) to find

$$y/y_0 = \left(\frac{\epsilon}{2} + \sqrt{\frac{\epsilon^2}{4} + \frac{T^2}{8}}\right)^{1/3} - \left(\sqrt{\frac{\epsilon^2}{4} + \frac{T^2}{8}} - \frac{\epsilon}{2}\right)^{1/3}, \qquad (15)$$

where $y = p - p_F$ and $y_0 = (3Mp_F/v_2)^{1/3}$. With these results, the integrals I_k are calculated numerically that yields

$$L_{\rm QCP}(0)/L_0 = 1.81 \ . \qquad (16)$$

Thus close to the QCP, the ratio $L_{\rm QCP}(0)/L_0$ is enhanced as compared with the FL value (3). This result is in agreement with the experimental value of the violation of the WF law, observed in Refs. 10,13.

d. Numerical calculations of the Lorenz number $L(T)$ through the topological QCP. In this paragraph we show results of numerical calculations of Eq. (13) with an interaction function f, having the analytical form

$$f(q) = \frac{\lambda}{(q^2/4p_F^2 - 1)^2 + \alpha^2} \ , \qquad (17)$$

where the parameter λ is fixed, while the parameter α, depending on r_s, is chosen to provide the best agreement with the microscopic spectrum, drawn in Fig. 1. Results of calculations of the momentum distribution $n(p,T)$ and spectrum $\epsilon(p,T)$ at different values of α are given in the second and third columns of Fig. 2 respectively. On the FL side, (the upper panels (a) and (b)), of the QCP, located at $\alpha = 0.479$, the spectrum $\epsilon(p,T)$ has the standard FL form (2) that holds until the effective mass M^* attains values $\simeq 10^2 M$. The QCP spectrum $\epsilon_c(p,T)$, with the group velocity $v_F(T)$ vanishing at $T = 0$ is shown in the third panel (c). It differs from the FL one in two aspects. First, at $T \to 0$ it has the inflection point. Second, its form drastically changes with T elevation.

Having at hand the spectrum $\epsilon(p)$, the transport integrals (6) are straightforwardly evaluated. Results of calculations of the functions $L(T)$ and $K(T) = 3I_2(T)/(\pi^2 I_0(T))$ are shown in the first column of Fig. 2. The upper panel (a) of Fig. 2 illustrates the situation on the FL side of the QCP ($\alpha = 0.520$, $M^*/M = 6$). We observe no deviations from the FL predictions. As seen from the panel (b), the WF law also holds in the immediate vicinity of the QCP ($\alpha = 0.482, M^*/M = 80$). However, the departure from FL theory, associated with the temperature dependence of the spectrum $\epsilon(p,T)$, becomes well pronounced in both the ratios $K = 3I_2/(\pi^2 I_0)$ and $S = I_1/I_0$ already at extremely low $T \simeq 10^{-3}\epsilon_F^0$. The QCP results are shown in the middle panel (c). We see that the WF law is, indeed, violated: the ratio $L(0)/L_0$ turns out to be in excess of 1, in agreement with the above result (16).

Results, shown in two lower panels (d) and (e), where $\alpha = 0.475$ and $\alpha = 0.472$ correspondingly, demonstrate that as the system goes away from the QCP, the value of the group velocity $v_F(T = 0)$ turns out to be finite again, and the WF law (3) is recovered. However, already at $T \simeq 10^{-4}\epsilon_F^0$, even lower, than on the FL side, the Lorenz number $L(T)$ becomes $T-$dependent.

e. Topological phase transitions in strongly correlated Fermi systems. As seen from the panels (d) and (e), beyond the QCP, equation

$$\epsilon(p) = \mu \qquad (18)$$

has three roots $p_1 < p_2 < p_3$, the curve $\epsilon(p, T = 0)$ crosses the Fermi level three times, and occupation numbers $n(p, T = 0)$ become: $n(p) = 1$ at $p < p_1$, while at $p_1 < p < p_2$, $n(p) = 0$; at $p_2 < p < p_3$, once again $n(p) = 1$, and at $p > p_3$, $n(p) = 0$. Thus at the coupling constant $g > g_{\rm QCP}$, the Fermi surface becomes multiconnected. This is a typical topological phase transition, at which no one symmetry, inherent in the ground

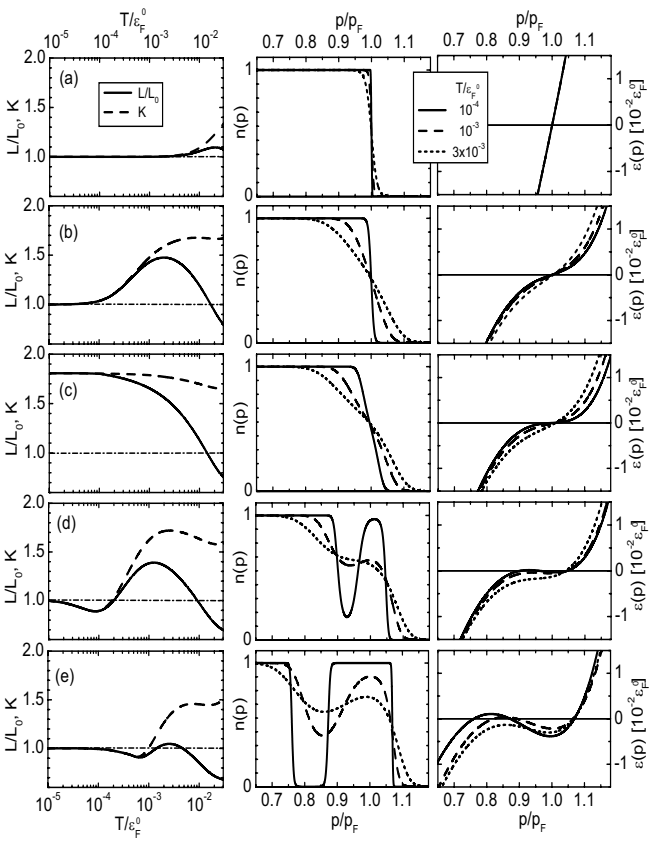

FIG. 2: The reduced Lorenz number $L(T)/L_0$ together with the ratio $K(T) = 3I_2(T)/(\pi^2 I_0(T))$ (left panels) as functions of the reduced temperature T/ϵ_F^0, the occupation numbers $n(p)$ (middle panels) and the single-particle spectrum (right panels) calculated at different line-type-coded temperatures with the interaction function (17) for five different sets of input parameters, which correspond to five different cases: Fermi liquid with the effective mass $M^*/M \simeq 6$, i.e. quite far from the QCP (panels a); Fermi liquid with $M^*/M \simeq 80$, which is close to the QCP (panels b); system at the QCP (panels c), the state just beyond the QCP, with $p_2 - p_1 \simeq 0.14\, p_F$ (panels d) and the state well beyond the QCP, with $p_2 - p_1 \simeq 0.31\, p_F$ (panels e).

state, is violated.[30,31,32,33] As the interaction strength increases, the number of the points, where the spectrum $\epsilon(p, T = 0)$ crosses the Fermi level, rapidly grows, however, the number of roots of Eq. (18) remains countable.

In another type of the topological transitions, the so-called fermion condensation,[34,35,36,37,38,39] the roots of Eq. (18) form an uncountable set. Indeed, the ground state energy E is a functional[1,2] of the quasiparticle momentum distribution $n(p)$, confined within the interval $0 < n < 1$. In the strong coupling limit, the minimum of this functional is found from the variational condition[34]

$$\frac{\delta E}{\delta n(p)} = \mu, \quad p \in \mathcal{C} \ , \qquad (19)$$

the chemical potential μ, being determined by the requirement $\sum n(p) = \rho$. Since the l.h.s. of Eq. (19) is

nothing but the quasiparticle energy $\epsilon(p)$, we see that in the case at issue, solutions of Eq. (18), called the fermion condensate (FC), exist in a whole domain $\mathcal{C}$, giving rise to swelling of the Fermi surface. Remarkably, the presence of the FC results in breaking of the *particle-hole symmetry*, another salient feature of the phenomenon of fermion condensation, that exhibits itself in a marked violation of the WF law.

True, if the interaction strength is small, the solutions of Eq. (19) do not meet the restriction $n(p) \leq 1$. However, beginning with a critical constant, i.e. at $g > g_{\rm FC}$, these solutions, *smooth* functions $n_*(p)$, meet this restriction wherever. Thus on the Lifshitz phase diagram, the FL phase occupies a region $g < g_{\rm QCP}$, a domain $g_{\rm QCP} < g < g_{\rm FC}$ is occupied by the phase, having the multi-connected Fermi surface, while a domain $g > g_{\rm FC}$, by the FC phase.

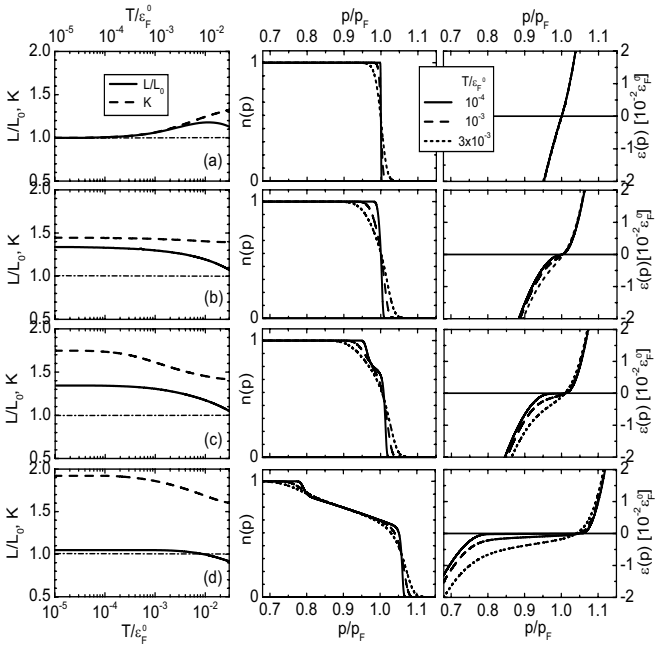

FIG. 3: Same as in Fig. 2 calculated with the interaction function (20) for $\beta p_F = 3$ and four values of the parameter g in units of M^{-1}: 3.0 (Fermi liquid, panels a), 3.55 (QCP, panels b), 3.9 (the state with the FC fraction $\rho_{\rm FC}/\rho = 0.1$, and 4.8 (the state with $\rho_{\rm FC}/\rho = 0.5$, panels d).

f. Breaking of the particle-hole symmetry and the WF law in systems with a fermion condensate. It is worth noting that if the interaction function $f(q)$ possesses a singularity at $q = 0$, then the Lifshitz phase diagram, constructed above, alters, since the phase with the multi-connected Fermi surface disappears, and at $g > g_{\rm QCP}$ the system contains the normal quasiparticles and a FC fraction that grows linearly with the difference $g - g_{\rm QCP}$. This situation is convenient for the demonstration of the impact of breaking of the particle-hole symmetry in systems with a FC on the violation of the WF law. In what follows we address a model with the interaction function

$$f(q) = g \exp(-\beta q)/q \ . \tag{20}$$

The structure of the FC, emerging at $g > g_{\rm QCP}$, is found with the help of formulas, given in Ref. 36. It is shown in Figs. 3 and 4. As seen from Figs. 3 and 4, the model derivative $dn(p)/dp$ has peaks at both the boundary points of the FC region. Notably vicinities of these points contribute overwhelmingly to the transport integrals I_k, since the single-particle spectrum $\epsilon(p, T = 0)$ identically vanishes inside the FC domain. Outside this domain,[36]

$$\frac{d\epsilon(p, T = 0)}{dp} \propto \sqrt{|\epsilon(p)|} \ . \tag{21}$$

This power behavior results in a marked violation of the WF law. Indeed, upon inserting Eq. (21) into Eq. (6) one finds that major contributions to every of the integrals I_k, proportional to $T^{1/2}$, come from the exterior of the FC domain, while its interior ensures minor ones, proportional to T. This conclusion is confirmed by results of numerical calculations, shown in Fig. 5

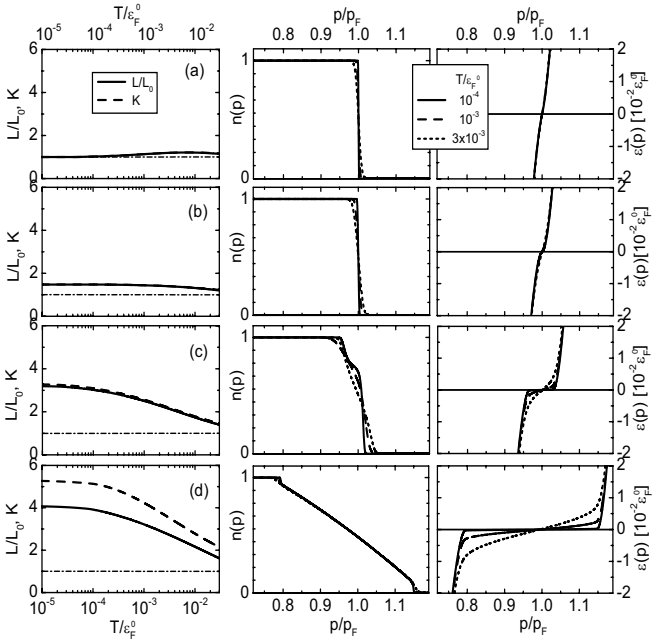

FIG. 4: Same as in Fig. 3 calculated for $\beta p_F = 30$ and four values of the parameter g in units of M^{-1}: 25.0 (Fermi liquid, panels a), 33.4 (QCP, panels b), 69.0 (the state with $\rho_{\rm FC}/\rho = 0.1$, panels c), and 224.0 (the state with $\rho_{\rm FC}/\rho = 0.5$, panels d).

The transport integrals I_k are calculated numerically. In Fig. 5, we show results of these calculations, performed with the value of the dimensionless parameters $\beta p_F = 3$ and $\beta p_F = 30$. As seen from this figure, at the QCP and beyond it the integrals $I_0(T = 0)$ and $I_1(T = 0)$ has the same order, implying that in contrast

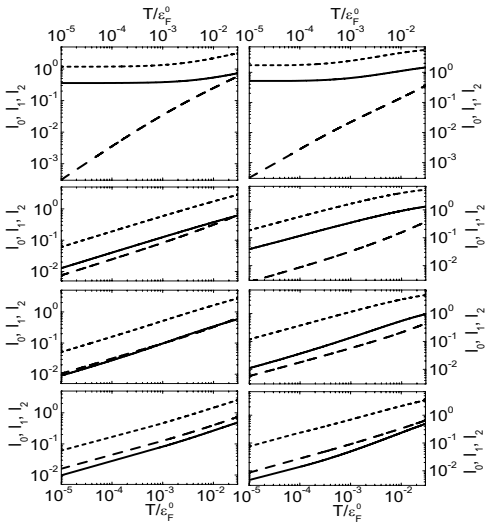

FIG. 5: The transport integrals I_0 (solid lines), I_1 (dashed lines) and I_2 (short-dashed lines) in log-log scale as functions of reduced temperature T/ϵ_F^0, calculated with the interaction function (20) for $\beta p_F = 3$ (left column) and $\beta p_F = 30$ (right column) and four values of the parameter g corresponding to FL (upper panels), the QCP (second line of panels), and to the states with 10% (third line) and 50% (lower panels) of quasiparticles in the FC.

to FL theory, the $T = 0$ value of the Seebeck coefficient $S(0) = I_1(0)/eI_0(0)$ differs from 0, an exhibition of breaking of the particle-hole symmetry, occurring in any system with a FC. On the other hand, the ratio $L(0)/L_0$ turns out to be even larger than at the QCP. Furthermore, calculations demonstrate that with increasing β, the value of this ratio increases as well, i.e. the longer the radius of the interaction function (20) in the coordinate space, the larger is the departure from the WF law.

g. Anisotropy of the violation of the WF law close to the QCP in heavy-fermion metals. The anisotropic Fermi surface of the majority of heavy-fermion metals has a sector, where at $T \to 0$, the quasiparticle group velocity v_F keeps a finite value, implying that the WF law holds. However, recently in experimental studies of $CeCoIn_5$ in external magnetic fields, close to the critical value H_c, suppressing superconductivity of this metal, the WF law was found to be violated.[12] The violation is anisotropic that cannot be attributed to the collapse of collective degrees of freedom. On the other hand, close to the topological QCP, the conductivity tensors $\sigma_{ik} \propto <v_i v_k>$ and $\kappa_{ik} \propto <\epsilon(\mathbf{p}) v_i v_k>$ become anisotropic, and this anisotropy is well pronounced in sufficiently large magnetic fields. Indeed, the magnetic field does not affect the $z-$components of the velocity $\mathbf{v}$, parallel to its direction. As a result, the particular QCP T-dependence of the integrals I_k holds, triggering the violation of the WF relation $L_{zz} = \sigma_{zz}/(T\kappa_{zz}) = \pi^2/3e^2$. On the other hand, the electron motion is completely rearranged in the direction, perpendicular to $\mathbf{H}$ that leads to a considerable increase of the respective components of the group velocity and the suppression of the departure of the respective components of the ratio $\mathbf{L}$ from their WF value.

h. Conclusion. In conclusion, we have demonstrated that flattening of single-particle spectra $\epsilon(p)$ of strongly correlated electron systems considerably changes their transport properties, especially beyond the point of fermion condensation due to breaking of the particle-hole symmetry. Results of our analysis demonstrate that search for the violation of the WF law in new materials should be confined to electron systems without disorder, possessing, nevertheless, a sufficiently large resistivity, the fact, justifying a minor role of light carriers. One more distinguished feature of systems, where marked departures from the WF law can exist, is related to the enhancement of the Seebeck coefficient $S(T \to 0)$ and the ratio $q(T \to 0) = eS(T \to 0)/C(T \to 0)$. Interestingly, these features are inherent in the heavy–fermion metals where the violation of the WF law was observed. Indeed, in CeNiSn, the q value exceeds 10^2.[19] Its value is markedly enhanced in compounds $Pr_{2-x}Ce_xCuO_{4-y}$ as well.[40]

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